Emergent Collective Modes and Kinks in Electronic Dispersions

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Recently, it was shown that strongly correlated metallic fermionic systems [Nature Phys. **3**, 168 (2007)] generically display kinks in the dispersion of single fermions without the coupling to collective modes. Here we provide compelling evidence that the physical origin of these kinks are emerging *internal* collective modes of the fermionic systems. In the Hubbard model under study these modes are identified to be spin fluctuations, which are the precursors of the spin excitations in the insulating phase. In spite of their damping, the emergent modes give rise to signatures very similar to features of models including coupling to external modes.

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The description of nascent collective modes which emerge from elementary excitations on varying a control parameter g is an intensely studied field of research. The difficulty relies on the fact that in one limit of g the elementary excitations dominate while in the other limit the collective modes dominate. In the vicinity of the transition or around the crossover necessarily both degrees of freedom need to be taken into account so that the interplay of both kinds of excitations is crucial. No simple theory assesses this interplay.

Here we will focus on strongly correlated electronic systems and especially on the metal-insulator transition induced by a repulsive interaction U on a lattice with a commensurate number of electrons per site. The simplest case is a local interaction with one electron per site on average [1]. For low values of U the electrons move through the lattice so that the system is metallic. For large values of U the hopping is blocked and the system is insulating with frozen charge degree of freedom. However, the spin dynamics is still active. In the leading order in t/U (t, the hopping matrix element), this dynamics is captured by a Heisenberg model [2]. The collective modes are the spin excitations built from bound electron-hole pairs.

When the system is still metallic, but close to its insulating regime, we intend to understand how the emergent spin modes influence the electronic quasiparticles. This issue is important to many strongly correlated systems. One prominent example is high-temperature superconductivity where a large number of theories explains the attractive interaction between charge carriers by the interplay with spin fluctuations. One line of argument links the kinks that are observed in the dispersion of the fermionic holes (see for instance [3–7]) to the interaction with bosonic modes. This is the usual reasoning for phonons coupled to electrons [8]. Other bosonic modes, however, will engender the same sort of kinks, for instance plasmons [9]. In the high-T_c materials, spin fluctuations have an important influence on the quasiparticles; see, e.g., Ref. [10]. They are likely candidates for the bosonic modes; see, e.g., Ref. [11] where this is worked out in the fluctuation-exchange approximation.

Byczuk *et al.* [12] recently showed by a sophisticated analysis of the equations of dynamic mean-field theory (DMFT) [1] that kinks in the electronic dispersion are a generic feature of strongly correlated electronic systems where the repulsive interaction is of similar strength as the kinetic energy. They stress that no coupling to a bosonic mode is needed. Indeed the model they study does not comprise any explicit bosonic mode; it is a fermionic Hubbard model. For particle-hole symmetric models dominated by the local self-energy the position of the kink was related by Byczuk *et al.* [12] to the quasiparticle weight

$$\omega_{\mathrm{kink}} = (\sqrt{2} - 1)ZD. \quad (1)$$

In the present work it is our aim to elucidate the physical origin of the kinks. We provide evidence that the kinks result from the coupling to the bosonic resonance which is the precursor of the spin modes in the insulator. Thus we conjecture that the kinks in strongly correlated fermionic systems are induced by coupling to *internal* bosonic modes. The signature is very similar to the coupling to external bosons such as phonons [8]. Our finding also sheds light on signatures of spin modes in the electronic dispersions of high-temperature superconductors.

Our computation is also based on DMFT. This approach reduces the extensive lattice problem to a self-consistency problem involving a single-impurity Anderson model (SIAM) [1]. The latter can be viewed as an interacting site coupled to a semi-infinite chain of noninteracting fermions [13,14] , which is solved by dynamic density-matrix renormalization (D-DMRG) [15,16]. This combination of D-DMRG and DMFT represents a powerful tool for investigating the $T = 0$ one-particle propagators of interacting lattice models [17–20]. Its particular merit is to have a well-controlled energy resolution over the whole energy range [15,21].

The model under study is the simplest, displaying an interaction driven metal-insulator transition, namely, the half-filled Hubbard model

$$\mathcal{H} = -t \sum_{\langle i,j\rangle;\sigma} \hat{c}^{\dagger}_{i;\sigma}\hat{c}_{j;\sigma} + U\sum_{i}(\hat{n}_{i;\uparrow} - 1/2)(\hat{n}_{i;\downarrow} - 1/2). \tag{2}$$

At low values of U the ground state is metallic; above $U_{c2} \approx 3D$ the insulating phase becomes the ground state [1,19,22,23].

Our analysis is facilitated by the direct numerical calculation of the local proper self-energy $\Sigma(\omega)$. This is done with the help of the improper self-energy

$$Q(\omega) := \langle\langle \hat{d}_{\sigma}(\hat{n}_{-\sigma} - 1/2)|(\hat{n}_{-\sigma} - 1/2)\hat{d}^{\dagger}_{\sigma}\rangle\rangle, \tag{3}$$

where we use the notation $\langle\langle A|B\rangle\rangle$ for the Fourier transform of the time-dependent fermionic Green function $-i\langle\{A(t), B(0)\}\rangle$. If one considers doping, the term 1/2 in (3) is to be replaced by the average filling per site.

Starting from the result $\Sigma(\omega) = UF(\omega)/G(\omega)$ by Bulla *et al.* [24], we apply the Liouville operator in the equations of motion once more [25], yielding $F(\omega) = UQ(\omega)G_0(\omega)$ wherein $F(\omega) := \langle\langle \hat{d}_{\sigma}(\hat{n}_{-\sigma} - 1/2)|\hat{d}^{\dagger}_{\sigma}\rangle\rangle$. Substituting $F(\omega)$ by $UQ(\omega)G_0(\omega)$ and expressing $G(\omega)$ by Dyson's equation $G^{-1}(\omega) = G^{-1}(\omega) - \Sigma(\omega)$ yields

$$\Sigma(\omega) = U^2Q(\omega)/(1 + U^2Q(\omega)G_0(\omega)). \tag{4}$$

This expression is advantageous to use for small to moderate values of $U \lesssim 2D$ where the computation of $\Sigma(\omega)$ from the difference between the inverse bare and full propagators is numerically not reliable [20].

Figures 1 and 2 display the generic behavior found for U not too far from the metal-insulator transition. Figure 1(a) shows that a kink in the real part of a self-energy is linked to a troughlike feature in the imaginary part. This is a purely mathematical fact stemming from Kramers-Kronig relation. Figure 1(b) depicts the real and imaginary parts for a realistic self-energy as it results from the DMFT calculation. The kinks in the real part and the trough in the imaginary part are clearly discernible though not as neatly as in the analytic function of Fig. 1(a). This comes from small spurious wiggles in $-\mathrm{Im}\Sigma$ resulting inevitably from the deconvolution of the DMRG raw data [26].

In Fig. 2 we address the physical meaning of the troughlike feature. There are two ways to understand it based on Fermi-liquid theory.

(i) The trough itself, ranging approximately from $-0.1D$ to $0.1D$, is fitted by a narrow curve (dash-dotted line). Outside the trough $-\mathrm{Im}\Sigma(\omega)$ is then much lower than the extrapolated fit. Since $-\mathrm{Im}\Sigma(\omega)$ is the decay rate for

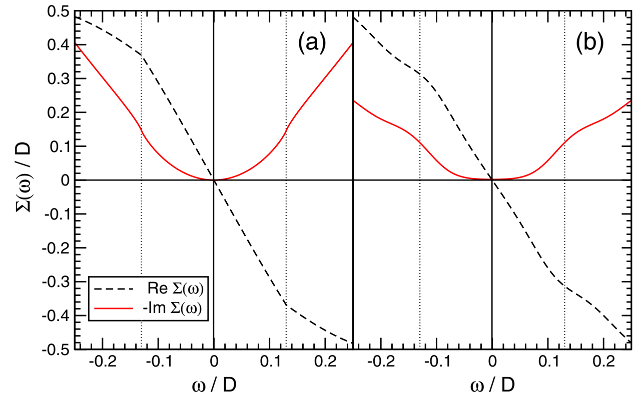

FIG. 1 (color online). Panel (a) illustrates the relation between real and imaginary parts for an analytic ansatz of the real part with a kink: $\mathrm{Re}\Sigma = \frac{-A^2}{2}\frac{(2\omega+|\omega-a|-|\omega+a|)(\omega^2-b^2)}{A^2+\omega^4}$, with $A \approx 0.62177D$, $a = 0.15D$, $b = 0.7D$; the imaginary part is computed by the Kramers-Kronig relation. Panel (b) shows the real and imaginary parts of $\Sigma(\omega)$ in DMFT at $U = 2.0D$.

the quasiparticles, this would be much lower relative to its extrapolated value. We do not see a good reason for such a decrease of the decay because the decrease due to reduced phase space for three quasiparticles should occur beyond about 3 times $ZD/2$, which is $\approx 0.4D$ [19,20,22], i.e., significantly larger than the extension of the trough.

(ii) The Fermi-liquid theory extends to higher values, for instance $\approx 0.5D$ as is still consistent with the above crude estimate, so that fits such as the dashed curve in Fig. 2 are justified. Indeed, the fit works very nicely with a moderate coefficient for the quartic term. This view implies that around $0.15D$ *additional* decay becomes possible, which extends up to $0.4D$. An additional decay channel is well possible. It sets in only above a certain energy because excitations of a certain minimum energy are involved.

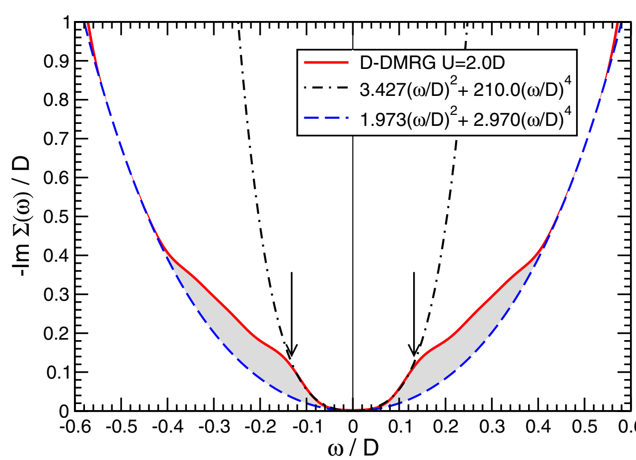

FIG. 2 (color online). $-\mathrm{Im}\Sigma(\omega)$ on a larger scale with two Fermi-liquid fits. The shaded region illustrates additional decay indicated by the arrows.

So, among the two hypotheses we favor the second one. It explains also rather naturally why the quadratic coefficient is so low in spite of the very narrow trough.

We are aware that from a puristic point of view on Fermi-liquid theory its applicability ends at the borders of the narrow trough as described above in (i). We do not claim that this view is invalid. But we advocate the alternative view (ii) because it provides an intuitive way to understand the self-energy behavior at low energies in terms of quasiparticles coupled to emergent collective modes. This coupling is the origin for the deviations from the dashed curve in Fig. 2. The latter is regarded as an effect on top of the underlying Fermi-liquid description resulting from the additional decay channel. This is induced by scattering from an emergent collective mode which has to be identified.

Given the fact that it becomes important only for finite, though small energies, we aim for a mode that is dominated by such a finite, though small energy. Furthermore, it exists only close to the metal-insulator transition. We shall see that its energy decreases towards the transition $U \rightarrow U_{c2}$. Because the insulator is a paramagnet with disordered local spin moments [1,27], a natural candidate is the emergent spin fluctuations.

In the framework of the limit of infinite dimension $d \rightarrow \infty$ the propagation of a collective mode from site i to site j scales as $d^{-|i-j|}$, where $|\cdots|$ stands for the taxi cab metric. Hence the collective modes are almost dispersionless and thus local. Only for particular wave vectors, which are of measure zero, can a nonlocal propagation make itself felt; see, e.g., Ref. [28]. In the complex diagrams describing the single particle motion the propagation of collective modes (particle-hole pairs) occurs in such a way that it is summed over. No particular momenta of measure zero matter. Thus it is fully sufficient to investigate the local response.

In Fig. 3 the local spin susceptibility $\chi_{\mathrm{spin}}(\omega)$ is shown, which we have computed for positive frequencies denoting it by $\chi^{>}_{\mathrm{spin}}(\omega)$. It is obtained from the effective SIAM occurring in the self-consistency loop of the DMFT [1,20]. In the SIAM it is determined as the local susceptibility at the head of the chain. Numerically we employ again D-DMRG for some broadening η, which is then eliminated by deconvolution [26]. This deconvolution gives rise to some uncertainty in the shape of the frequency dependence of the susceptibility.

The excitation operator is $2S^z = \hat{n}_\uparrow - \hat{n}_\downarrow$ at the chain head. A strongly pronounced peak catches the eye. Its peak energy moves towards $\omega = 0$ for $U \rightarrow U_{c2}$. In parallel, its height increases such that its total weight tends to a finite value [27]. This peak is the precursor of a δ peak at zero energy in the paramagnetic insulator. There it reflects the fact that a spin can be rotated without any cost of energy. Still in the metallic phase, the peak is a resonance made from an almost bound quasiparticle and a hole. It has some width because it may decay into scattering states of its constituents.

From the data for $\mathrm{Im}\chi^{>}_{\mathrm{spin}}$ we deduce the peak position by fits assuming two Lorentzians to account for the asymmetry of the peak shape. The Lorentzians are multiplied by factors $\tanh(\omega/\omega_0)$ to account for the linear vanishing of $\mathrm{Im}\chi^{>}_{\mathrm{spin}}(\omega)$ for $\omega \rightarrow 0$. The relevant peak position is the one of the Lorentzian with more weight. The error bars account for the uncertainties related to the details of the fit procedure, e.g., for $U \approx 1.9D$ where the weight appears to be distributed equally over both Lorentzians.

The results are compared in Fig. 4 with the kink positions which were determined in several ways. We use

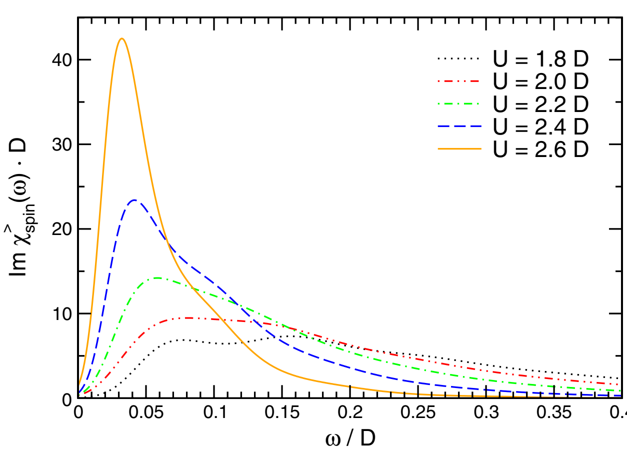

FIG. 3 (color online). Deconvolved imaginary part of the local spin susceptibility at positive frequencies for various interactions U in the metallic phase.

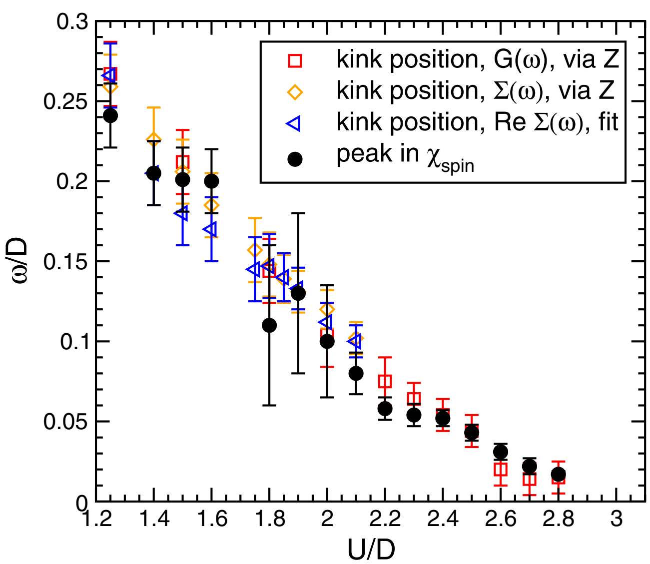

FIG. 4 (color online). Kink positions ω_{kink} as derived from the quasiparticle weight Z via Eq. (1); Z is found from either the propagator G [19] or the self-energy $\Sigma(\omega)$ in $Z = (1 - \partial_\omega \Sigma(0))^{-1}$. Most directly, a fit $A\omega + B(|\omega - \omega_{\mathrm{kink}}| - |\omega + \omega_{\mathrm{kink}}|)$ to $\mathrm{Re}\Sigma(\omega)$ is used for ω_{kink}; ω_{kink} is compared to the energies where $\chi^{>}_{\mathrm{spin}}$ shows a peak at low $|\omega|$.

Eq. (1) to deduce the kink position from Z, which in turn is determined by either $Z = [1 - \partial_\omega \Sigma(0)]^{-1}$ or $Z^{-1} = D^2 \partial_\omega G(0)/2$ [19]. Or the kink position is determined directly by a fit to $\mathrm{Re}\Sigma(0)$ (see caption of Fig. 4). The three ways to find the kink positions agree very well providing consistent data.

The peak positions agree remarkably well with the kink positions. For large values of U, in particular, the agreement is striking. It is for these larger values $U \gtrsim 2D$ that both the kink and the peak in the susceptibility are clearly discernible and well defined. So we deduce that the additional decay channel seen in Fig. 2 results from the excitation of the spin resonance by the propagating single fermionic quasiparticle. This finding strongly supports our claim that the kink is in fact due to emergent internal modes. Here these modes are the spin fluctuations which develop already in the metallic phase.

Thereby, an intuitive physical picture of the origin of the kinks is found. One major advantage of this picture is that one can transfer it to finite dimensions where the collective modes are dispersive so that the momentum dependence matters. Kinks are to be expected where momentum and energy conservation for the scattering of a quasiparticle from a collective mode is fulfilled.

In conclusion, we have provided compelling evidence for a link between the kinks in fermionic dispersions in strongly correlated systems and emergent internal collective modes, spin fluctuations in particular. We agree completely with the phenomenon established by Byczuk *et al.* [12]. But our physical picture of the phenomenon is different because we view the kinks as the consequence of inherent bosonic modes. An important concomitant aspect is that the Fermi-liquid theory does not break down already at the scale of ω_{kink}. It extends to about $2ZD$, where Z is the quasiparticle weight.

Our finding provides important information on the possible interpretation of kinks in electronic dispersions in many strongly correlated systems and in cuprate systems as they occur in high-temperature superconductors in particular. Such kinks can be the consequence of emerging bosonic modes, i.e., resonances even if these are still strongly damped. For instance, qualitative support is provided to results based on the fluctuation-exchange approximation for cuprates [11]. Moreover, the coupling between the single particles and the collective modes is generically substantial. Certainly, further investigations, for instance away from half filling, are called for.

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